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# Thermo-kinetics characterization of kerosene/RP-1 combustion

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#### THERMO-KINETICS CHARACTERIZATION OF KEROSENE/RP-1 COMBUSTION\*

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#### Abstract

A one-formula surrogate fuel C<sub>12</sub>H<sub>24</sub> and its quasiglobal kinetics have been developed to support the conceptual design of the injectors and thrust chambers of the tri-propellant engines. This surrogate fuel represents a fuel blend that properly depicts the physical and chemical properties of kerosene/RP-1. The accompanying thermodynamics for the substitute fuel is generated and is anchored with the heat of formation of kerosene/RP-1. The surrogate fuel model and its thermodynamics are verified by comparing a series of one-dimensional rocket thrust chamber thermo-equilibrium calculations under a kerosene-fueled Russian Engine (RD-170) operating conditions. The models are then tested in conjunction with a computational fluid dynamics formulation to predicting the thermo-flowfield of two single-element shear tri-axial injectors: a gaseous oxygen-kerosenehydrogen injector and a liquid oxygen-liquid kerosenegaseous hydrogen injector. The mixture ratio of those injectors is that of a proposed tri-propellant engine RD-704. Reasonable flame structure is predicted for those injectors.

### Introduction

Russian-built kerosene-fueled rocket engines such as RD-170 or its U.S. proposed counterparts such as RD-704 and Bantam have been identified as potential candidates to fly the Single-Stage-to-orbit Reusable Launch Vehicles. In order to support the associated engineering issues, specifically the preliminary conceptual design and evaluation of the propellant injectors and thrust chambers using Computational Fluid Dynamics (CFD), accurate and computationally efficient models that properly represent the fuel formula,

thermodynamics, and combustion kinetics have to be used. Unfortunately, models pertaining to those aspects were underdeveloped.

An elemental formula, CH<sub>1,9423</sub>, and its derived standard heat of formation have been used in oneperformance dimensional theoretical rocket calculations for JP-4/RP-1 powered engines. However, they can not be used for elevated inlet temperatures since other thermodynamic properties were amiss, and they can not be used in the more elaborate CFD calculations since fuel molecular formula has to be used. A molecular formula C<sub>10</sub>H<sub>19</sub> was listed<sup>2</sup> for kerosene but its molecular weight is too low. Another formula C<sub>12</sub>H<sub>23</sub> was used as kerosene<sup>3</sup>. However, it is a radical and its H/C ratio is too low. Ref. 4 performed a one-dimensional calculation using a major component n-dodecane (C<sub>12</sub>H<sub>26</sub>) to represent RP-1 in a 77-reaction kinetics set. However, n-dodecane is a paraffin whose H/C ratio is too high and the rates that were used to decompose C<sub>12</sub>H<sub>26</sub> to major fragments and acetylene were unjustified. In addition, the assumption of RP-1 as 100% paraffin led to erroneous selection of a slow soot formation mechanism<sup>5</sup>, while in actuality the approximately 56% cyclic naphthene and 3% aromatics in RP-16 should command a fast condensation polymerization route to soot formation.

In this study, based on reported physical-chemical property data, a one-formula surrogate fuel  $C_{12}H_{24}$  is proposed as a general representation for kerosene and its derived fuels, RP-1 in particular. Its heat capacity, enthalpy and entropy were generated from 300K to 5,000K and the rationale for generation is given. The surrogate fuel model and its thermochemical properties are verified by comparing a series of one-dimensional

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rocket thrust chamber shifting-equilibrium calculations for a kerosene-fueled Russian engine (RD-170). The computed chamber and nozzle exit temperatures and species compositions from the proposed model compared very well with those of using elemental formulas CH<sub>2</sub> and CH<sub>1.9423</sub>. A kerosene/RP-1 combustion kinetics is also proposed based on a quasi-global kinetics format. The final thermo-kinetics model is coupled with a CFD formulation to compute the thermo-flowfield of two single-element, tri-propellant, tri-axial injectors.

#### One-Formula Surrogate Fuel Model

Common hydrocarbon rocket fuels such as kerosene, or jet fuels are derived from petroleum, while RP-1 is a straight run kerosene fraction<sup>6,7</sup>. Those hydrocarbon fuels are complex mixtures of many components and their exact composition and properties vary from batch to batch. Some qualitative information on those substances are available. For example, it is reported<sup>3</sup> that kerosene typically consists of ten hydrocarbons containing 10-16 carbon atoms per molecule, while the constituents include n-dodecane, alkyl derivatives of benzene, naphthalene and its derivatives. Also, 87 identifiable hydrocarbons is found in RP-18. A typical characterization of kerosene and RP-1 is shown in the first two columns of Table 1. A molecular formula can not be given since both fuels are complex blends, but some averaged molecular weights are reported. Averaged elemental formula and formula weight are also reported for RP-1. Some heat of combustion data and limited heat capacity data are given. A heat of formation was derived for CH<sub>1,9423</sub>. **Typical** composition of RP-1 is 41% paraffins, 56% naphthenes, 3% aromatics, and no olefins.

It is obvious that a fuel model can not possibly account for all 87 hydrocarbons in RP-1, or even ten species for kerosene. A rational compromise would be to devise a surrogate fuel which is a neat compound or a mixture of a few neat components that best describes or approximate the thermo-chemical properties of the actual fuel, as described in Table 1. Such simplification is necessary when complex fuel blends are in question. In this study, a one-formula surrogate fuel,  $C_{12}H_{24}$ , is proposed as the general molecular representation for kerosene/RP-1. The advantage of this one-formula representation is that it does not have to be called a certain molecule, rather it represents either a neat compound or a mixture of many neat components that has the same averaged molecular formula and the right As a neat compound, e.g., pentylcomposition. methylcyclohexane (C<sub>12</sub>H<sub>24</sub>) in which a fusion of two

molecules can be envisioned: methylcyclohexane  $(C_7H_{14}, a naphthene)$  and pentane  $(C_5H_{12}, a paraffin)$ from which the carbon numbers give a paraffin-tonaphthene ratio of 41.6:58.3. As a mixture of two neat components, e.g., it can be seen as a mixture of ndodecene (C<sub>12</sub>H<sub>24</sub>) and pentyl-methylcyclohexane (C<sub>12</sub>H<sub>24</sub>) blended at a paraffin-to-naphthene ratio of 41.6:58.3, or a mixture of any other neat molecules with the same formula (C<sub>12</sub>H<sub>24</sub>) and the same paraffin-tonaphthene split. The resulting properties of the surrogate fuel as proposed is shown in the third column of Table 1. The molecular weight, elemental formula and formula weight, and the paraffin/naphthene split of the surrogate fuel matched closely with those of kerosene and RP-1. The paraffin-to-naphthene split is important to match if soot formation is to be accurately modeled. The small amount of aromatics and olefins in kerosene and RP-1 are ignored and lumped into the paraffins and naphthenes of the surrogate fuel model.

#### Surrogate Fuel Thermodynamics Generation

The first and most important thermodynamic property to be considered for the surrogate fuel is the heat of formation if accurate heat release during combustion is to be predicted. In general, the heat of formation can not be measured directly but must be determined indirectly from its heat of combustion, measurable calorimetrically. A combustion reaction for a general hydrocarbon fuel  $C_nH_m$  can be represented as:

$$C_nH_m + (n + 0.25 \text{ m})O_2 = n CO_2 + 0.5 \text{ m} H_2O$$

The heat of reaction of the above equation is the heat of combustion. By definition, the net heat of combustion is obtained when the product  $H_2O$  is at its gaseous state. The heat of formation of the general hydrocarbon is written:

$$H_{f,CnHm} = n H_{f,CO2} + 0.5 m H_{f,H2O} - H_{c}$$

To determine the heat of formation, a molecular formula must be specified and the heat of combustion measured. The flexibility of the one-formula surrogate fuel makes it unnecessary to determine the heat of formation from that of pentyl-methylcyclohexane, or n-dodecene, but directly from the reported heating values of kerosene/RP-1. Several reported standard heat of combustions are listed in Table 1. The maximum difference among them is only 0.115 kcal/g which amounts to about 1% of the heating value. These values are deemed as consistent among themselves and are within the uncertainty bound of the measurement. A

value of -10.278 kcal/g is hence chosen due to its midrange. As a result, a thermodynamically consistent heat of formation of -92.200 kcal/mole is derived for  $C_{12}H_{24}$  and a value of -7.683 kcal/mole is calculated for its elemental form  $CH_{2.0}$ , as shown in Table 1.

The next step is to construct the three thermodynamic functions of heat capacity, enthalpy, and entropy as functions of temperature in a usable form. The standard two-temperature, fourth-order polynomial form<sup>1</sup> is used:

$$\begin{split} &\frac{C_p}{R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ &\frac{H_T}{RT} = a_1 + \frac{a_2}{2} T + \frac{a_3}{3} T^2 + \frac{a_4}{4} T^3 + \frac{a_5}{5} T^4 + \frac{a_6}{T} \\ &\frac{S_T}{R} = a_1 \ln T + a_2 T + \frac{a_3}{2} T^2 + \frac{a_4}{3} T^3 + \frac{a_5}{4} T^4 + a_7 \end{split}$$

Due to the closeness of n-dodecane (C12H26) with C<sub>12</sub>H<sub>24</sub> family of molecules in terms of carbon and hydrogen atomic numbers and the notion<sup>3,8</sup> that ndodecane is a major component in kerosene/RP-1, the enthalpy of the surrogate fuel is constructed using the heat capacities of n-deodecane, but anchored with the thermodynamically consistent heat of formation of kerosene. This procedure is similar to that of Ref. 3 in which the enthalpy of n-dodecane was used as a placeholder. The surrogate fuel heat capacity matched well with the available data, as indicated in Table 1. The entropy of formation of n-dodecane, in a less important sense, is also used to construct the entropy curve. The resulting least square coefficients fitted for two temperature ranges are listed in Table 2. While the original intent was to generate a vapor phase thermodynamics for temperatures above the normal boiling point (542 K)6, the fitted thermochemical properties started from the standard state temperature, i.e., 298.15 K. The state of the surrogate fuel at temperatures below normal boiling point, in a practical sense, can be viewed as either liquid or hypothetical gas. This is justified since the value of the heat of vaporization (0.059 kcal/g at normal boiling point)<sup>6</sup> is not only much smaller than that of the heat of combustion, but also is less than the error bound (0.115 kcal/g) of the heat of formations<sup>1,2,6,7</sup>. In addition, the latent heat decreases to zero at critical pressure, as most of the rocket engines are operated at higher pressures. This gives the current model an added advantage over CH<sub>1,9423</sub><sup>1</sup> in that fuel inlet temperatures above 298.15 K

can be treated. Nonetheless, different sets of thermochemical coefficients can be regenerated for vapor phase and/or liquid phase according to the same procedure if more reliable data are found and improved accuracy is needed.

#### Surrogate Fuel Thermodynamics Validation

A one-dimensional theoretical rocket engine performance calculation was performed for the proposed one-formula kerosene/RP-1 surrogate fuel model and its thermodynamics. The thrust chamber specifications and operating conditions were those of a Russian engine RD-170<sup>9,11</sup>. Fig. 1 shows a comparison of the calculated theoretical chamber and nozzle exit temperatures as a function of mixture ratios for C<sub>12</sub>H<sub>24</sub>, CH<sub>2</sub>, and CH<sub>1,9423</sub>. The calculated temperatures for C<sub>12</sub>H<sub>24</sub> and CH<sub>2,0000</sub> coincide, as expected, since their heat of formations are consistent with the chosen heat of combustion at -10.278 kcal/g. Also shown in Fig. 1, are the results using elemental formula CH<sub>1.9423</sub> with heat of formations of -5.430, -6.613, and -7.133 kcal/mole. These values correspond to heat of combustions of - $10.356^{1}$ ,  $-10.278^{7}$ , and  $-10.241^{6}$  kcal/g, respectively. The difference among the curves is small since the difference in heat of combustions is considered small, especially in fuel lean region. When based on the same heat of combustion, the minor temperature difference between CH<sub>2</sub> and CH<sub>1.9423</sub> comes from the difference in H/C ratios.

Fig. 2 shows the predicted theoretical nozzle exit gas composition. Again, the mole fractions of  $C_{12}H_{24}$  coincide with those of  $CH_{2.000}$ . Graphite carbon and methane gas formed at nozzle exit at low mixture ratios due to fuel rich combustion at low exit temperatures, as expected. These results showed that one-formula kerosene/RP-1 surrogate fuel model and its thermodynamics model are suitable for theoretical rocket performance calculations.

#### **Quasi-Global Combustion Kinetics**

Detailed kinetics mechanism involving elementary steps is computationally prohibitive for considering kerosene/RP-1 combustion in CFD calculations. On the other hand, one-step<sup>3</sup> or multiple-step global kinetics models<sup>12</sup> is computationally efficient, but often not generic enough to take advantage of the modern diagnostic techniques. For example, hydroxyl radical (OH) is usually not involved in those models and laser-induced fluorescence imaging of the OH-radical flame structure data<sup>13</sup> can not be utilized. The quasi-global

kinetics which is a bridge between the detailed mechanism and the one-step to multiple-step global kinetics is probably best suited for describing complex fuel combustion in a computationally intensive environment. The original quasi-global kinetics<sup>14</sup> was established based on the observation that straight-chain hydrocarbons hydrocarbons and cyclic different ignition delay distinctively time characteristics, and that the ignition delay times for straight chain hydrocarbons are similar and so are the ignition delay times for the cyclic hydrocarbons. This important observation paves the way for the development of the quasi-global kinetics model: a irreversible global step using a generic rate that breaks down the straight chain hydrocarbons into CO and H<sub>2</sub> and another irreversible global step with a separate generic rate that combusts the cyclic hydrocarbon into the same intermediate products, and a detailed CO-wet mechanism that converts the CO to CO<sub>2</sub> and H<sub>2</sub> to H<sub>2</sub>O.

OH radical is not only considered in the wet mechanism, but plays a vital part in the accurate prediction of the heat release during combustion. This original quasi-global kinetics scheme<sup>14</sup> was evaluated in a variety of flow configurations, including stirred reactors, plug flows, and turbulent diffusion flames with swirl. It was later expanded to an "extended" quasiglobal kinetics model<sup>15</sup> which include two more intermediate species (C<sub>2</sub>H<sub>2</sub> and C<sub>2</sub>H<sub>4</sub>) and several more global kinetic steps to better describe the fuel-rich combustion. In this study, though, under the premises of computational efficiency and the framework of oneformula surrogate fuel model, format of the original quasi-global kinetics is considered. Following that format, two global steps are proposed: one for the paraffin portion and another for the naphthene part of the surrogate fuel. The rates of the two global steps are modified directly from those of the straight chain and cyclic global steps14 according to the paraffin and naphthene split of the proposed surrogate fuel model  $(C_{12}H_{24})$ . The proposed reactions and rates of those two global steps along with the reactions and forward rates for the CO-wet mechanism are shown in Table 3. The "stoichiometric" in the "Form" column means it is calculated as the multiplication of the reactant concentrations raised to the power of their respective stoichiometric coefficients. The backward rates of those reversible reactions are calculated from their respective forward rates and equilibrium constants.

Under fuel rich conditions, kerosene/RP-1 forms soot readily. Naphthene and aromatic hydrocarbons are known to form soot rapidly by direct condensing to polycyclic aromatic hydrocarbons (PAH), while paraffins

form soot slowly by breaking into smaller fragments from which fusing occurs and PAH's form indirectly. These PAH's, also known as soot precursors, are then undergone a series of physical processes to form coagulated soot particles. A comprehensive soot formation model involving approximately elementary reversible reactions and 180 species has been formulated in an attempt to describe the aforementioned soot formation processes. It is far too expensive to be incorporated into a CFD code at the present moment, let alone the oxidation of those 180 species. A global step making soot directly from C<sub>12</sub>H<sub>24</sub> is proposed instead, as shown in Table 3. For convenience, graphite carbon (C<sub>s</sub>) is used to represent soot. The rates are modified from those established for toluene combustion in a jetstirred combustor<sup>15,18</sup> by multiplying the pre-exponential factor by (0.583\*6)<sup>1.81</sup>. The factor 6 converts the C<sub>12</sub>H<sub>24</sub> to that of equivalent acetylene since acetylene was used to represent the unburnt hydrocarbons in the original rate form<sup>18</sup>, while the factor 0.583 is the naphthene fraction in the one-formula kerosene/RP-1 fuel model.

The soot oxidation model is modified from that of Ref. 16. In Ref. 16, rates of carbon oxidation were measured for carbon filament, reactor graphite and pyrographite and fitted with a heterogeneous reaction model involving three elementary steps and two active carbon sites to forming CO. This work simplifies the three-step reactions to a one-step global kinetics, while maintaining the rates and the rate form for heterogeneous reactions, as shown in Table 3.

#### Application to Tri-Propellant Injectors

The proposed thermal-kinetics models are incorporated into a CFD code, FDNS<sup>19</sup>, for computing the thermo-flowfields of a hypothetical gaseous O<sub>2</sub>/kerosene/H<sub>2</sub> injector and a more realistic liquid O<sub>2</sub>/liquid kerosene/gaseous H<sub>2</sub> injector, hereon referred to as a GGG injector and a LLG injector, respectively. These are shear tri-axial injectors and are modified from those of Penn State's single element gaseous O2/H2 shear coaxial injectors 13 by adding a third injection slot. In this study, Oxygen injects from the center tube, while kerosene comes from the next annulus and hydrogen enters from the outermost annulus. Computationally, these single element injectors are housed in a throated ombustion chamber similar to Penn State's optically accessible rocket chamber<sup>13</sup>, in order to have a well defined downstream boundary condition while maintaining a nearly constant chamber pressure. Unlike Penn States's shear coaxial injector,

though, these injectors have no recessed post. The mixture ratio of the propellants and the operating conditions are similar to those of engine RD-704. This computation sets up an example for tri-propellant engine design calculations using CFD.

#### Numerical Algorithm

FDNS is a multidimensional, multispecies, viscous flow, pressure-based reacting flow solver. multiphase version<sup>20</sup> solves simultaneous liquiddroplets-gas dynamics by combining the volume-offluid (VOF) and Eulerian/Lagrangian tracking methods into a unified algorithm for efficient calculations of multiphase free surface and droplet flows at all speeds. The gas-liquid interface mass, momentum and energy conservation properties are modeled by continuum surface mechanisms. A unique feature of the current VOF method is that multispecies VOF has been formulated, hence liquid oxygen and liquid kerosene can be solved. In the VOF formulations, the weightaveraged conservation equations of mass, momentum, and scalar variables are casted in an Eulerian framework. Liquid energy equation solves temperature as the dependent variable, meaning it is not sensitive to the liquid species composition, rather the temperature difference and the transport process of the environment. Current formulation also ignores the liquid inter-species mass transport and the direct vaporization of liquids into gases. An empirical mass stripping rate is applied to the VOF equation along the liquid-gas interface for liquid intact core resolution. The stripped liquid mass undergoes secondary breakup process to form smaller droplets. Lagrangian particle tracking method is used to treat the dynamics and heat/mass transfer of droplets, as computational parcels in a statistical sense. Energy and momentums are solved for each parcel for every species and relative enthalpy is the dependent variable for the droplet energy equation. For simplicity, parcel temperature is assumed to be constant at any time instant, but varies throughout its life expectancy via local heat transfer at the surface and vaporization. The heat capacity and latent heat of vaporization for liquid kerosene were taken from Ref. 21.

## Results

The comparison of the temperature contours for GGG and LLG injectors is shown in Fig. 3. The grid is identical for both cases and the grid density is 149x69. To start the calculation, a cold-flow GGG injector flowfield was computed first until the nozzle flow at the end of the combustor choked. The propellants in the

mixing layers were then ignited by temporarily assigning a elevated temperature (1000 K) in a small flow domain between the side wall and the mixing layers. Once ignited, the flame propagates upstream and spreads downstream. The flow recirculation region near the backward-facing step formation of the injector faceplate holds the flame. After the flame structure in the GGG injector took shape, a separate LLG injector flowfield is computed by turning on the liquid oxygen and kerosene flows at their respective inlets. The standoff distance between the flame front and the injector faceplate of the LLG injector appears to be longer and the general temperature level appears to be lower than those of the GGG injector. The combustion takes place most vigorously in the mixing layers from which the expansion of the hot gases diverted portion of the torch toward the side wall. Fig. 4 shows the soot concentration contours for both cases. The soot yield of the GGG injector is higher than that of the LLG injector near the injector faceplate, primarily due to the higher temperature that raises the rate of soot formation. The predicted flame structures and flowfields looked reasonable.

#### Conclusion

A simplified thermo-kinetics model has been developed for tri-propellant engine design calculations. The model consists of a surrogate fuel model representing kerosene/RP-1 fuels, a thermodynamics model anchored with the heat of combustion, and a quasi-global kinetics model describing the combustion of kerosene/RP-1, including soot formation and oxidation reactions. The surrogate fuel and its thermodynamics models, by themselves, can be used to perform one-dimensional rocket engine performance calculations at elevated inlet fuel temperatures. Adding the quasiglobal kinetics, this thermo-kinetics model can be use in conjunction with CFD to predict the performance and thermo-flowfield for more detailed design applications.

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Table 1. Comparison of thermo-chemical characterization of model fuel with reported data.

	Kerosene	RP-1	Kerosene/RP-1 surrogate fuel model
Molecular Formula			$C_{12}H_{24}$
Molecular Weight	175 <sup>9</sup>	172-175 <sup>6</sup>	168
Elemental Formula		CH <sub>1.95</sub> -CH <sub>2.0</sub> <sup>6</sup> , CH <sub>1.9423</sub> <sup>1</sup> , CH <sub>1.953</sub> <sup>9</sup>	CH <sub>2.0</sub>
Formula Weight		13.97-14.03 <sup>6</sup> ,13.97 <sup>1</sup>	14.03
H <sub>c</sub> , kcal/g	-10.278 <sup>7</sup> ,	-10.241 <sup>6</sup> ,	-10.278
	-10.321 <sup>2</sup>	-10.356 <sup>1</sup>	
H <sub>f,298K</sub> , kcal/mole		-5.430 <sup>1</sup> /CH <sub>1.9423</sub>	-92.200/C <sub>12</sub> H <sub>24</sub> ,
			-7.683/CH <sub>2.0</sub>
C <sub>p,516k,1 atm</sub> , cal/mole-K		1016	103
Paraffins (n and iso) %		416	41.7
Naphthenes %		56 <sup>6</sup>	58.3
Aromatics %	5 <sup>7</sup>	5 <sup>10</sup> ,3 <sup>6</sup>	0
Olefins %	17	06	0

Table 2. Thermodynamic coefficients for  $C_{12}H_{24}$ .

	1000 to 5000 K	300 to 1000 K
a <sub>1</sub>	0.36440206E+02	0.39508691E+01
a <sub>2</sub>	0.54614801E-01	0.10207987E+00
a <sub>3</sub>	-0.16091151E-04	0.13124466E-04
a <sub>4</sub>	0.21478497E-08	-0.76649284E-07
a <sub>5</sub>	-0.10131180E-12	0.34503763E-10
a <sub>6</sub>	-0.63890109E+05	-0.52093574E+05
a <sub>7</sub>	-0.15798973E+03	0.21980951E+02

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Table 3. Kerosene/RP-1 quasi-global combustion kinetics mechanism.  $K_f = AT^B e^{-E/RT}$ .

Reaction_	A	В	E/R	Form	Ref.
Paraffin Global Step					
$C_{12}H_{24} + 6O_2 \rightarrow 12CO + 12H_2$	3.888E4	1	1.220E4	$p^{0.3}[C_{12}H_{24}]^{0.5}[O_2]$	This Work
			}		
Naphthene Global Step				0.5	}
$C_{12}H_{24} + 6O_2 \rightarrow 12CO + 12H_2$	2.132E7	1	1.965E4	$p^{0.3}[C_{12}H_{24}]^{0.5}[O_2]$	This Work
Wet CO Mechanism	1.700512		0.40754	C444	14.15
$H_2 + O_2 = OH + OH$	1.700E13	0	2.407E4	Standard	14,15
$OH + H_2 = H_2O + H$	2.190E13	0	2.590E3	Standard Standard	14,15
$OH + OH = O + H_2O$	6.023E12	_	5.500E2	1	14,15
$O + H_2 = H + OH$	1.800E10 1.220E17	1.0 -0.91	4.480E3 8.369E3	Standard Standard	14,15 14,15
$H + O_2 = O + OH$	1.000E16	0.91	0.309E3	Standard	14,15
M + O + H = OH + M	2.550E18	-1.0	5.939E4	Standard	14,15
$M + O + O = O_2 + M$	5.000E15	0.1.0	3.939E4 0	Standard	14,15
$M + H + H = H_2 + M$	8.400E21	-2.0	0	Standard	14,15
$M + H + OH = H_2O + M$	4.000E12	0	4.030E3	Standard	14,15
$CO + OH = H + CO_2$	3.000E12	0	2.500E4	Standard	14,15
$CO + O_2 = CO_2 + O$	6.000E13	ŏ	2.50024	Standard	14,15
$CO + O + M = CO_2 + M$	0.000213	"	U	Standard	14,15
Soot Formation Global Step					į į
	1.1935E16	-1.94	1.610E4	$[C_{12}H_{24}]^{1.81}[O_2]^{-0.5}$	This Work
$C_{12}H_{24} \rightarrow 12C_s + 12H_2$	,		2.01027	[0]224] [02]	
Soot Oxidation Global Step					
$C_s + 0.5O_2 \rightarrow CO$	1.0	0.	0.	$72R_{ox}[C_s]/(\rho_sD_s)$	This Work
$C_s + 0.5C_2 \rightarrow CC$				0A1 05 (, 0 0)	
$R_{ox} = K_A p_{O2} \chi / (1 + K_Z p_{O2})$					16
$+ K_{B}p_{O2}(1-\chi)$					
$\chi = 1/(1 + (K_T/K_B)p_{O2})$	2 000051		1 500051		
K <sub>A</sub>	2.0000E1	0	1.5098E4		
K <sub>B</sub>	4.4600E-3	0	7.6497E3		
K <sub>τ</sub>	1.5100E5	0	4.8817E4		
K <sub>z</sub>	2.1300E1	υ	-2.063E3		

<sup>\*</sup> M stands for third-body collision partner

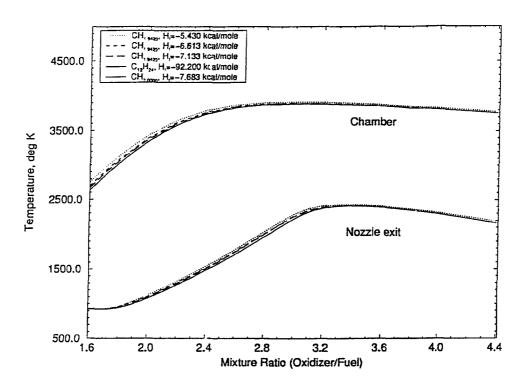


Fig. 1 Comparison of the RD-170 chamber and nozzle exit temperatures.

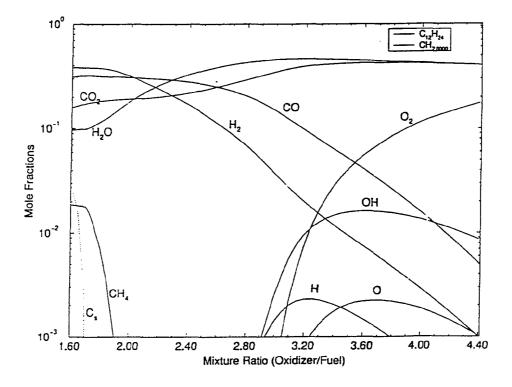


Fig. 2 The RD-170 nozzle exit gas composition.

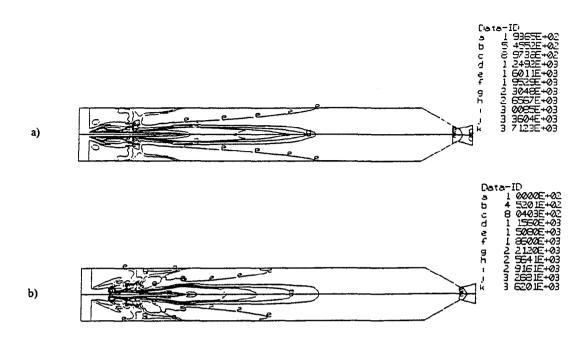


Fig. 3 Comparison of the temperature contours for a) GGG and b) LLG injectors.

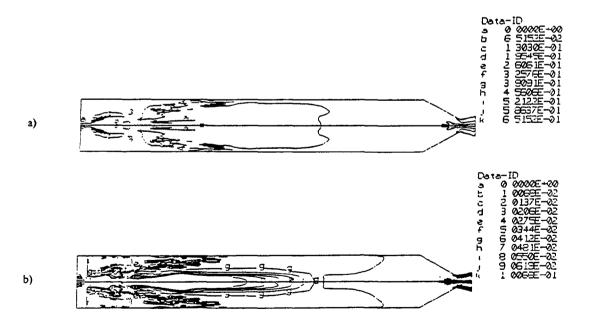


Fig. 4 Comparison of the soot mass fraction contours for a) GGG and b) LLG injectors.